Integrative Structure Validation Report

July 22, 2024 - 05:19 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	9A3E
PDB-Dev ID	PDBDEV_00000199
Structure Title	Structure of SH3 domain from chicken alpha spectrin determined using restraints from solid-state NMR
Structure Authors	Soeldner B; Grohe K; Neidig P; Auch J; Blach S; Klein A; Vasa S K; Schafer L V; Linser R

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

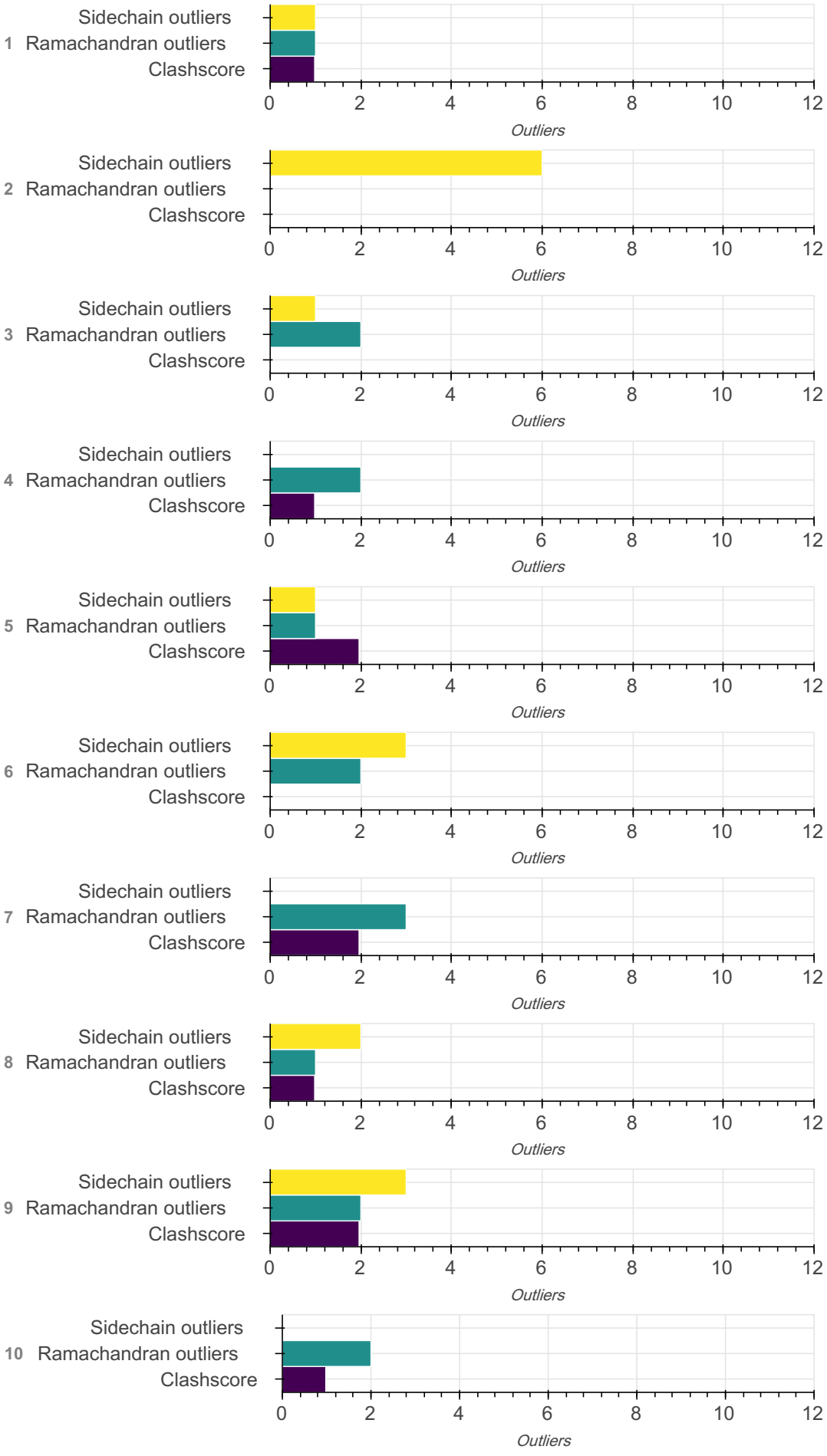
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

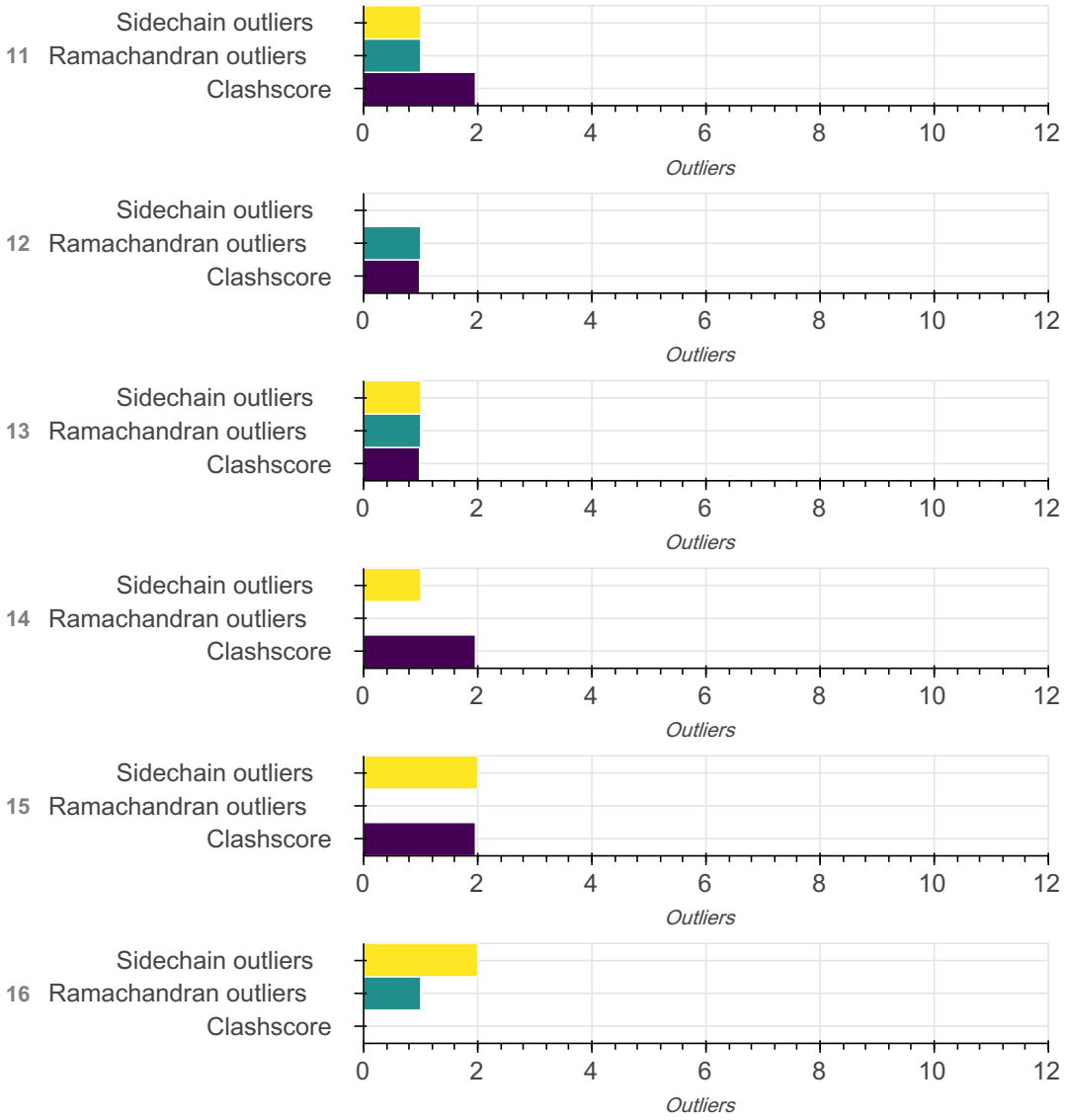
List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis


1
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
2
4
6
8
10
12
Outliers



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 16 unique models, with 1 subunits in each model. A total of 4 datasets or restraints were used to build this entry. Each model is represented by 0 rigid bodies and 3 flexible or non-rigid units.

Entry composition

There are 16 unique types of models in this entry.These models are titled Final model of replica 1, Final model of replica 2, Final model of replica 3, Final model of replica 4, Final model of replica 5, Final model of replica 6, Final model of replica 7, Final model of replica 8, Final model of replica 9, Final model of replica 10, Final model of replica

11, Final model of replica 12, Final model of replica 13, Final model of replica 14, Final model of replica 15, Final model of replica 16 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	spectrin alpha chain	A	A	62
2	1	1	spectrin alpha chain	A	A	62
3	1	1	spectrin alpha chain	A	A	62
4	1	1	spectrin alpha chain	A	A	62
5	1	1	spectrin alpha chain	A	A	62
6	1	1	spectrin alpha chain	A	A	62
7	1	1	spectrin alpha chain	A	A	62
8	1	1	spectrin alpha chain	A	A	62
9	1	1	spectrin alpha chain	A	A	62
10	1	1	spectrin alpha chain	A	A	62
11	1	1	spectrin alpha chain	A	A	62
12	1	1	spectrin alpha chain	A	A	62
13	1	1	spectrin alpha chain	A	A	62
14	1	1	spectrin alpha chain	A	A	62

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
15	1	1	spectrin alpha chain	A	A	62
16	1	1	spectrin alpha chain	A	A	62

Datasets used for modeling

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	2NUZ
2	Experimental model	PDB	6SCW
3	NMR data	BMRB	34785
4	Experimental model	PDB	8CF4

Representation

This entry has only one representation and includes 0 rigid bodies and 3 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-6, 7-61, 62-62

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Restrained Molecular Dynamics Simulation	modeling	None	256000	False	False

There is 1 software package reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	GROMACS	2019.2	model building	http://www.gromacs.org

Data quality

NMR

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	0.98	1
2	0.00	0
3	0.00	0
4	0.98	1

Model ID	Clash score	Number of clashes
5	1.96	2
6	0.00	0
7	1.96	2
8	0.98	1
9	1.96	2
10	0.98	1
11	1.96	2
12	0.98	1
13	0.98	1
14	1.96	2
15	1.96	2
16	0.00	0

All 18 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:3:GLU:O	A:6:LYS:HE3	0.432
4	A:30:ILE:N	A:30:ILE:HD12	0.437
5	A:25:MET:HE1	A:58:VAL:HG13	0.451
5	A:43:LYS:HE2	A:50:GLN:HB3	0.413
7	A:33:LEU:CD2	A:60:LYS:HE2	0.522
7	A:33:LEU:HD23	A:60:LYS:HE2	0.421
8	A:23:VAL:HG12	A:49:ARG:CZ	0.511
9	A:13:TYR:CG	A:14:ASP:N	0.408
9	A:10:LEU:HB2	A:61:LEU:HD21	0.401

Model ID	Atom-1	Atom-2	Clash overlap (Å)
10	A:39:LYS:HE3	A:40:ASP:OD2	0.539
11	A:33:LEU:CD2	A:60:LYS:HE2	0.566
11	A:33:LEU:HD22	A:60:LYS:HE2	0.417
12	A:41:TRP:CZ3	A:54:PRO:HD3	0.487
13	A:42:TRP:CH2	A:60:LYS:HE3	0.583
14	A:9:VAL:HG23	A:31:LEU:HB2	0.419
14	A:22:GLU:HA	A:52:PHE:O	0.405
15	A:33:LEU:CD2	A:60:LYS:HE3	0.426
15	A:8:LEU:HD23	A:32:THR:HA	0.415

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	60	55	4	1
2	60	55	5	0
3	60	54	4	2
4	60	54	4	2
5	60	54	5	1
6	60	54	4	2
7	60	53	4	3
8	60	59	0	1
9	60	56	2	2
10	60	57	1	2
11	60	55	4	1

Model ID	Analyzed	Favored	Allowed	Outliers
12	60	56	3	1
13	60	56	3	1
14	60	56	4	0
15	60	57	3	0
16	60	55	4	1

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	56	50	5	1
2	56	49	1	6
3	56	49	6	1
4	56	50	6	0
5	56	50	5	1
6	56	48	5	3
7	56	53	3	0
8	56	49	5	2
9	56	53	0	3
10	56	54	2	0
11	56	54	1	1
12	56	53	3	0
13	56	50	5	1
14	56	51	4	1
15	56	51	3	2

Model ID	Analyzed	Favored	Allowed	Outliers
16	56	49	5	2

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	58	VAL
2	A	1	MET
2	A	2	ASP
2	A	3	GLU
2	A	27	LYS
2	A	37	THR
2	A	58	VAL
3	A	14	ASP
5	A	38	ASN
6	A	3	GLU
6	A	23	VAL
6	A	25	MET
8	A	32	THR
8	A	58	VAL
9	A	4	THR
9	A	31	LEU
9	A	48	ASP
11	A	46	VAL
13	A	40	ASP
14	A	3	GLU

Model ID	Chain	Residue ID	Residue type
15	A	1	MET
15	A	30	ILE
16	A	32	THR
16	A	37	THR

Fit of model to data used for modeling

NMR

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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